

# The complexity of Platonic and Archimedean polyhedral links

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**Abstract** A mathematical methodology for understanding the complexity of Platonic and Archimedean polyhedral links has been developed based on some topological invariants from knot theory. Knot invariants discussed here include crossing number, unknotting number, genus and braid index, which are considered significant in view of DNA nanotechnology. Our results demonstrate that the braid index provides the most structural information; hence, it can be used, among four knot invariants, as the most useful complexity measure. Using such an invariant, it indicates that the complexity of polyhedral links is directed by the number of their building blocks. The research introduces a simple but important concept in the theoretical characterization and analysis of DNA polyhedral catenanes.

**Keywords** Platonic polyhedra · Archimedean polyhedra · Polyhedral links · Knot invariants · Complexity measures · DNA catenanes

## 1 Introduction

Complexity, a fundamental aspect of understanding many physical and biological systems, has become a current active subject in chemistry, and molecular complexity is one of the main issues in this fascinating topic [1]. To date, there are many attempts to define quantitative measures of complexity, which can be used to compare and classify

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various molecular graphs. In particular, the complexity of Platonic and Archimedean polyhedra have been examined by some well-known topological indices, such as the resistance distances [2–4], spanning trees [5,6], total walk counts [7,8], solid angles [9,10]. Fowler [4], Nikolic [5] and Fowler [6] are particular focused on a special type of polyhedra, called fullerenes.

In the past two decades, however, a variety of interlinked polyhedra with more exotic topologies have been synthesized. Using DNA molecules, experimental scientists have chemically realized five Platonic polyhedra including tetrahedron [11,12], cube [13–15], octahedron [16,17], dodecahedron [18], and icosahedron [19,20], as well as two Archimedean polyhedra containing truncated octahedron [21] and truncated icosahedron [18]. In the face of such topologically complex molecules with non-planar graphs, the description and quantification of their structural properties, involving entanglement complexity, appears to be of great chemical interest. The application of invariants from the mathematical technique of knot theory is novel and may prove to be a valuable untapped resource [22–25].

Scientists are aware of the importance of the topological complexity of knotted and linked molecules in 3-spaces and this has also been explored in some detail [26,27]. Until now, most of the studies are focused on some numerical methods from the point of view of knot physics, such as calculating writhe to understand the entanglement of polymers. The recent review article by Orlandini and Whittington [28] is an enjoyable exposition of this adventure.

On the other hand, if regardless of physical meaning, one regards DNA as a very thin string, then DNA polyhedra can be mathematically modeled as polyhedral links [29–32]. Here we will expose these mathematical objects to further scrutiny. Thus, some well known knot invariants such as crossing number, span of knot polynomials, unknotting number, braid index, genus and stick number, can be served as measures of their complexity [33–36]. In general, the larger of the measure of complexity, the more complex links. Although computation of these knot invariants can be very difficult, they play an important role in classifying and ordering distant knots and links.

The main goal of this paper is to discuss four knot invariants of Platonic and Archimedean polyhedral links. Research on crossing number, unknotting number, genus and braid index presents a new methodology for ordering the complexity among different polyhedral links. We also compare them with each other to find the most useful complexity measure. This idea of considering the complexity of polyhedral links is conceptually very simple; however, it provides a sound basis for the understanding of structures, properties and, further, the molecular design of DNA polyhedral catenanes.

## 2 Platonic and Archimedean polyhedral links

Platonic solids, polyhedra with all faces regular, are not only present in mathematics, but have attracted the attention of chemists as structural models time and again since antiquity [37]. There are five Platonic polyhedra: Tetrahedron (*T*), Cube (*C*), Octahedron (*O*), Dodecahedron (*D*) and Icosahedron (*I*).

Archimedean solids are semiregular polyhedra, which are resulted from Platonic solids by truncating or snubbing. Although their face degrees are not all the same, their

vertices are regular, i.e., the degrees of all of the vertices are same. They also build a rich treasure house for chemical molecules, for example, the famous fullerene  $C_{60}$  adopts the polyhedral shape known as the truncated icosahedron. There are thirteen Archimedean solids: Truncated tetrahedron (*Tt*), Truncated hexahedron (*Th*), Truncated octahedron (*To*), Truncated dodecahedron (*Td*), Truncated icosahedron (*Ti*), Cuboctahedron (*Cu*), Truncated cuboctahedron (*Tcu*), Snub octahedron (*So*), Rhombicuboctahedron (*R*), Icosidodecahedron (*Id*), Truncated icosidodecahedron (*Tid*), Snub icosidodecahedron (*Si*) and Rhombicosidodecahedron (*Ri*).

In [31], we introduced the method of ‘ $n$ -branched curves and  $m$ -twisted double-lines covering’ for constructing polyhedral links. Here, we modify the method of using ‘ $m$ -inverted twisted double-lines’ to instead of ‘ $m$ -twisted double-lines’ as edge building blocks. In this way, edges become antiparallel double-lines, whose orientation is consistent with the natural direction of DNA molecules. The other building blocks are  $n$ -branched curves, which are designed to cover vertices with  $n$ -degree. Connecting these building blocks can result in some oriented alternating polyhedral links, i.e., links with overcrossings alternating with undercrossings as one traverse a component in the direction. Applying the method to Platonic and Archimedean polyhedra can generate  $T_m$ -Platonic and Archimedean polyhedra links, whose diagrams are shown in Figs. 1 and 2. Note that, the twist number in each edge must be even to ensure the global direction, that is,  $m = 2k$  ( $k = 1, 2, 3 \dots$ ), and  $3 \leq n \leq 5$ , as the smallest and the largest vertex degree is 3 and 5, respectively. To simplify, all structures in Figs. 1 and 2 use two crossings to denote  $2k$  crossings on each edge, and reveal two outstanding properties: (1) Each face of polyhedra changes into a cyclic strand, which is linked  $2k$ -times to each of its neighbors. (2) Due to the appearance of twist structures, polyhedral links cannot be deformed to their mirror images, this is a property that they have topological chirality, which is detected by linking number [38,39].

### 3 Crossing number and unknotting number

The *crossing number* of a link  $L$ , denoted  $c(L)$ , is the least number of crossings that occur in any diagram of the link. It states that:

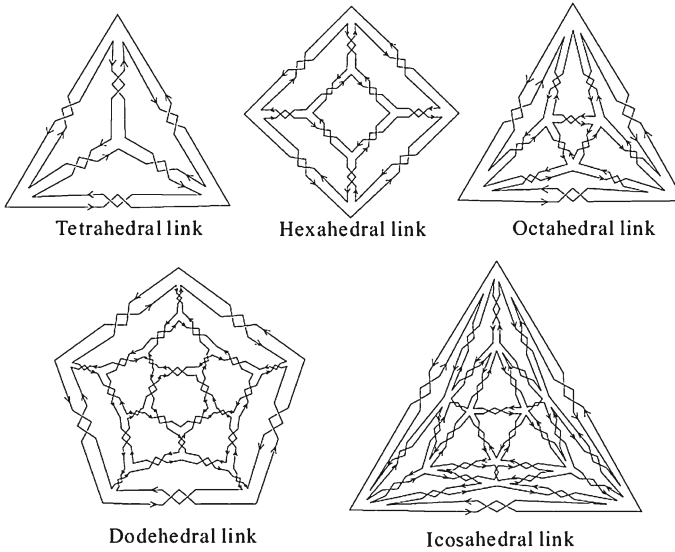
$$c(L) = \min\{c(D) : D \text{ is diagram of } L\}.$$

The determination of minimal diagram can be checked by the following lemma.

**Lemma 3.1** Sola [40] *Any alternating projection is minimal if and only if it does not contain an isthmus.*

Thus, a diagram  $D$  of a link is minimal if and only if it has no removed crossings. Fortunately, pictures in Figs. 1 and 2 are just minimal diagrams of Platonic and Archimedean polyhedral links. In our diagrams,  $2k$  crossings are distributed on each edge alternately. Since, it has been proved by Thistlethwaite [34] that an alternating link in a minimal diagram of  $n$  crossings has crossing number  $n$ . Thus, the equation of calculating their crossing numbers is given by:

$$c(L) = 2kE,$$



**Fig. 1** The diagrams of Platonic polyhedral links with minimal crossing numbers, where two crossings appeared on each edge represent  $2k$  twists

where  $E$  denotes the edge number of a polyhedron.

The *unknotting number* of a diagram  $D$  of a link, denoted  $u(D)$ , is the minimal number of crossing changes required to convert it into a diagram of the unlink. Then the unknotting number of a link  $L$  is denoted as  $u(L)$  and is also given by [41]:

$$u(L) = \min\{u(D) : D \text{ is diagram of } L\}.$$

Known as an unknotting operation, the crossing change means switching the over- and under-crossing strand at a crossing, which is shown in Fig. 3.

**Proposition 3.2** For a minimal diagram of a  $T_{2k}$ -polyhedral link shown in Figs. 1 and 2, the unknotting number  $u(D)$  is equal to  $kE$ , where  $E$  denotes edge number of the parent polyhedron.

*Proof* From a diagram of  $T_{2k}$ -polyhedral link, associate a vertex with each twist and connect two vertices with an edge if they are located in adjacent twists, thus, the relating planar graph  $G$  is obtained by replacing every edge of the polyhedron with the chain of length  $2k$ . See, for example, Fig. 4a shows a planar graph of  $T_2$ -tetrahedral link.

In graph theory, a crossing change corresponds to the operation of contracting (or deleting) a chain of length 2. If we change  $k$  crossings of every edges, i.e.,  $2k$  chain contracted to a vertex, then a graph  $G'$  with one vertex and  $F-1$  loops is obtained.  $G'$  is a connected graph without edges, i.e., an empty graph, as an example shown in Fig. 4b, and when turn it into a knot diagram give rise to an unlink. Thus, change  $kE$  crossings can untie the  $T_{2k}$ -polyhedral link.

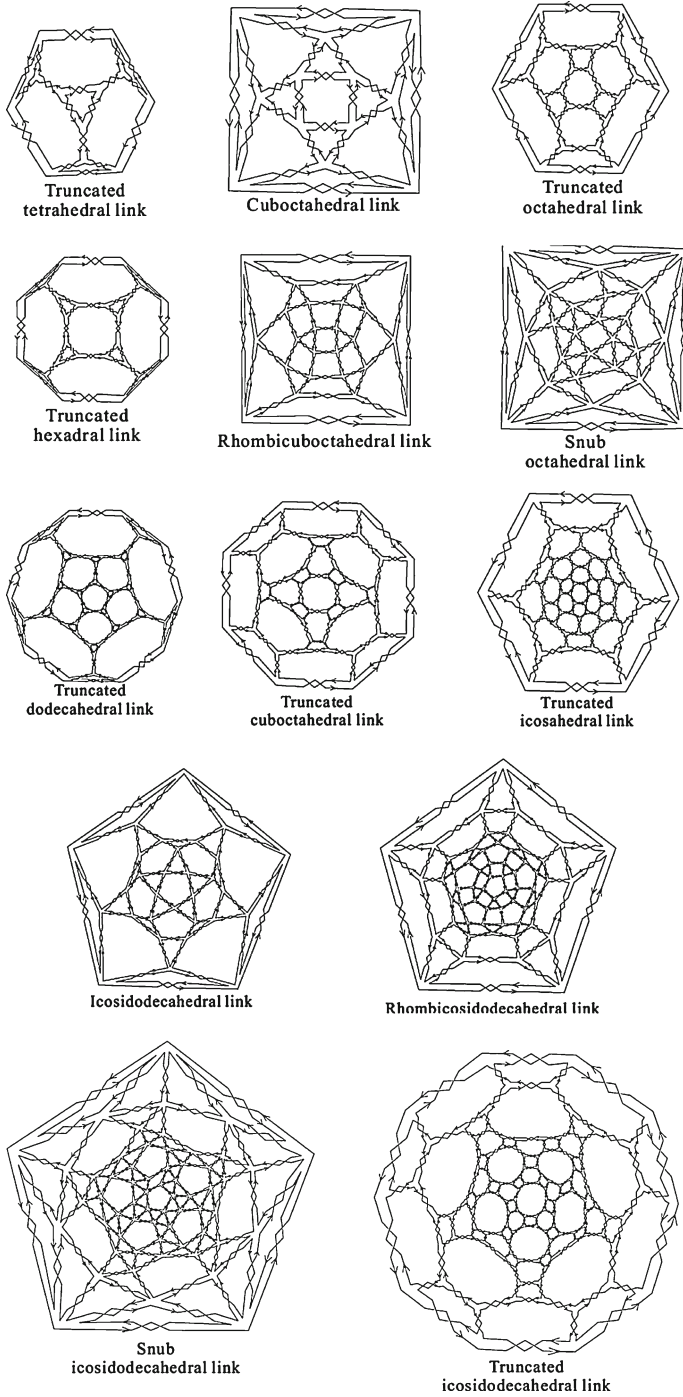
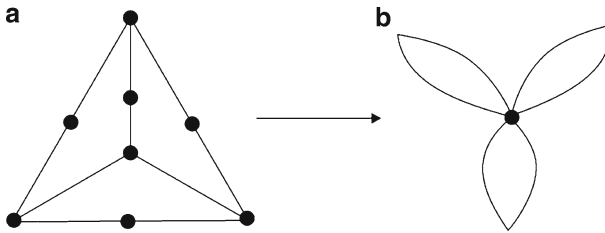
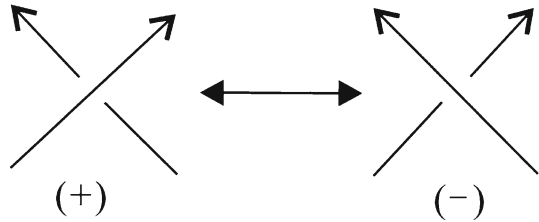


Fig. 2 The diagrams of Archimedean polyhedral links with minimal crossing numbers

**Fig. 3** The operation of crossing change



**Fig. 4** The progress of change a  $T_2$ -tetrahedral link graph into an empty graph by edge contraction

Now, there is a question of whether this number is the minimal. If we change less than  $kE$  crossings, then the resulting planar graph must contain an edge which is neither bridge nor loop. Suppose that the related link of such a graph is an unlink, then the graph has no edges except bridges. Thus, this contradiction shows that the result link is nontrivial. Thus, the number of crossing change  $kE$  is minimal, and  $u(D) = kE$ . This completes the proof.

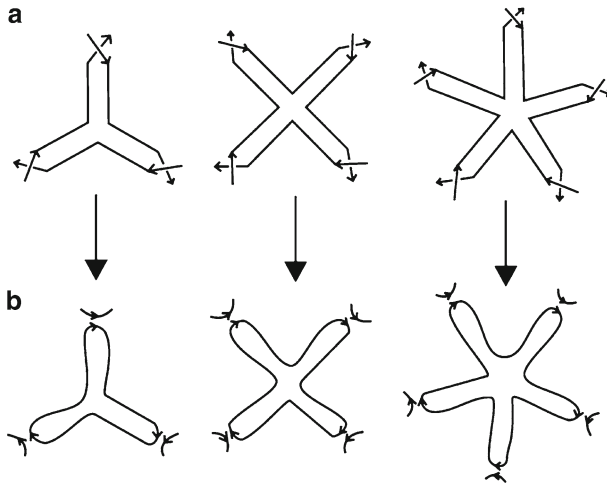
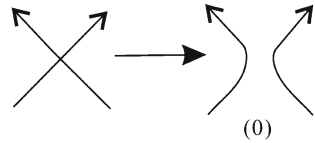
In fact, it is very hard to calculate the unknotting number of links  $u(L)$ , which can not be determined by the minimal number of crossing change on minimal diagrams. For example, the unknotting number  $u(L)$  of  $10_8$  in the Rolfsen table is realized by a non-minimal diagram [42]. Although we can not compute  $u(L)$  exactly, the unlinking number of diagrams  $u(D)$  can provides an upper bounds on  $u(L)$ ; that is, the unknotting number  $u(L)$  are less than or equal to  $kE$ .

Crossing number and unknotting number are mathematical important and also already have clear potential to be used in DNA nanotechnology. A crossing corresponds to a double-helical half-turn of DNA, which can act as a fundamental unit of DNA polyhedra. So, crossing number is a first-level order and relates to the structure of DNA polyhedra in solution. Unknotting number is equivalent to determining the minimum number of times needed for topoisomerase to mediate strand passage on a DNA polyhedral link to convert it into unlinked DNA circles.

#### 4 Genus and braid index

The *genus* of an oriented link  $L$ , denoted  $g(L)$ , is the minimum genus of any connected orientable surface that spans  $L$ . In order to calculating genus of links, we need to apply Seifert's algorithm to generate their Seifert surface. First, using the operation of crossing nullifying to a link, as shown in Fig. 5, a set of nonintersecting circles called *Seifert circles* will be generated. Then, connecting these circles each other at the

**Fig. 5** The operation of crossing nullifying



**Fig. 6** Applying crossing nullifying to vertex building blocks

position of link crossings by twisted bands, a *Seifert surface* with the link as boundary component is obtained. It has proved that every Seifert surface obtained by applying Seifert’s algorithm to alternating diagrams is of minimal genus [43].

**Proposition 4.1** *For a minimal  $T_{2k}$ -polyhedral link diagram shown in Figs. 1 and 2, the number of Seifert circles  $s(D)$  is equal to  $V + (2k - 1) E$ , where  $V$  and  $E$  are, respectively, the vertex and edge number of the parent polyhedron.*

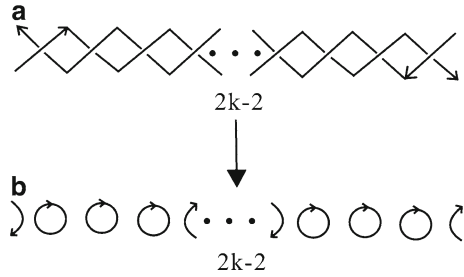
*Proof* A  $T_{2k}$ -polyhedral links can be decomposed into two building blocks, the vertex building block is  $n$ -branched curves with  $n$  additional crossings (Fig. 6a), and the other edge building block is  $2k-2$ -inverted twisted double-lines (Fig. 7a), where two crossings of each edge are assigned to vertices which it connected.

If apply the operation of crossing nullifying to a vertex building block, a  $n$ -branched curves with  $n$  additional crossings will yields  $1 + \frac{n}{2}$  Seifert circles, as shown in Fig. 6b. So, the number of Seifert circles derived from  $V$  vertices is  $(1 + \frac{n}{2}) V$ .

If apply the operation of crossing nullifying to a edge building block, a  $2k-2$ -inverted twisted double-lines can generates  $2k-2$  Seifert circles, as shown in Fig. 7b. So, the number of Seifert circles derived from  $E$  edges is  $(2k - 2) E$ .

Due to the additivity of Seifert circles,  $s(D) = (1 + \frac{n}{2}) V + (2k - 2) E$ , then followed by the relation  $2E = nV$  deduced by Euler formula:  $V + F - E = 2$ , we can conclude that:

**Fig. 7** Applying crossing nullifying to edge building blocks



$$s(D) = \left(1 + \frac{n}{2}\right) V + (2k - 2) E = V + (2k - 1) E.$$

This completes the proof.

Although the above proof is restricted to link diagrams in Fig. 1 and 2, the following conclusion of genus can be extended to any alternating diagram of polyhedral links. Applying the Seifert’s algorithm to any alternating diagram can produce a surface with minimal genus [43] and therefore the calculation of the genus is uniquely determined by whether the diagram is alternating.

Let us state the formula [35] for genus of an alternating link  $g(L)$ , which just is the genus of a diagram surface  $F$  constructed from a connected diagram  $D$  and satisfies:

$$2g(L) = [1 - s(D) + c(D)] + [1 - \mu(D)],$$

where  $s(D)$  denotes the number of Seifert circles,  $c(D)$  the number of crossing number,  $\mu(D)$  the number of component of diagram  $D$ .

In our cases,  $s(D) = V + (2k - 1) E$ ,  $c(D) = 2kE$ , and  $\mu(D) = F$ . Integrating these values into the equation in the above theorem, then we get:

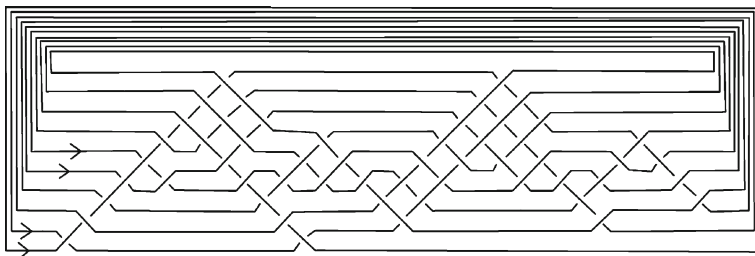
$$\begin{aligned} 2g(L) &= [1 - s(D) + c(D)] + [1 - \mu(D)] \\ &= 1 - V - (2k - 1) + 2kE + 1 - F \\ &= 2 - (V + F - E). \end{aligned}$$

By Euler formula  $V + F - E = 2$ , it leads to a surprising result that  $g(L) = 0$ .

A *braid* is a set of  $n$  strings intertwined each other that are attached to a horizontal bar both at the top and bottom. Each string always heads downward as we move along any one of the strings from the top bar to the bottom bar. It is clear that every link can be described by a closure of a braid [44], *i.e.*, pull the bottom bar around and glue it to the top bar. The *braid index* of link  $L$ , denoted  $b(L)$ , is the fewest number of strings needed to express  $L$  as a closed braid. For a particular diagram  $D$ , we proposed  $b(D)$  as the braid index of the link diagram, which means the number of strings needed to express  $D$  as a closed braid.

It is known by Yamada [45] that every diagram can be transformed into a closed braid with the number of Seifert circles unchanged. Thus, the braid index  $b(L)$  equals the minimum number of Seifert circles of all diagrams and  $b(D)$  equals the number of its Seifert circles, which provides an upper bound on  $b(L)$ . According to the above





**Fig. 8** The braid representation of the  $T_2$ -tetrahedral link

result of the number of Seifert circles, we easily have the braid index of  $T_{2k}$ -polyhedral link diagram  $b(D) = s(D) = V + (2K-1)E$ . As shown in Fig. 8, for example, the  $T_2$ -tetrahedral link can be represented by a ten-string braid.

Genus and braid index are also of substantial interest to modern chemistry and biochemistry. Genus, a topological invariant, is related to the Euler characteristics of the diagram and has been used to classify RNA structures [46]. Representing knotted hydrocarbon complexes as closed braids [47] can facilitate the study of their properties.

## 5 Discuss and conclusions

The present paper focuses on a complexity approach for polyhedral links based on four knot invariants. The values of crossing number, unknotting number, genus and braid index of Platonic and Archimedean polyhedral links are shown in Table 1.

In terms of crossing number and unknotting number as measures, the complexity of polyhedral links only depends on edge numbers of polyhedra. It is finding that crossing number are equal to  $2kE$ , and unknotting number  $u(D)$  are equal to  $kE$ , as linear functions of edge number  $E$ . Genus of all polyhedral links are zero, it means that Seifert surfaces of these links are homeomorphic to spheres with a set of discs removed. If consider genus as a complexity measure, it is trivial.

In contrast with three invariants motioned above, we show that the braid index  $b(D)$  is more powerful. From its calculating formula,  $V + (2k-1)E$ , we can see braid index  $b(D)$  that contains all the structural information of two building blocks, that is,  $V$  denotes the number of branched curves,  $E$  denotes the number of half-turn twists on double-lines. The complexity in terms of branched curves and double-lines is understood intuitively when we turn to a polyhedral graph, which means the more vertices and edges a graph is, the more complex it is. Translated back to chemistry, the braid index  $b(D)$  is relevant to the number of vertex and edge building blocks that a DNA polyhedron is needed. As seen in Table 1, the ordering of Platonic and Archimedean polyhedral links in terms of braid index  $b(D)$  is shown:  $T$ -links  $<$   $O$ -links  $<$   $C$ -links  $<$   $Tt$ -links  $<$   $Cu$ -links  $<$   $I$ -links  $<$   $D$ -links  $<$   $To$ -links =  $Th$ -links  $<$   $R$ -links  $<$   $Sc$ -links  $<$   $Id$ -links  $<$   $Tcu$ -links  $<$   $Ti$ -links =  $Td$ -links  $<$   $Ri$ -links  $<$   $Si$ -links  $<$   $Tid$ -links, close to the ordering of Platonic and Archimedean polyhedra. Moreover, for each link, the complexity will become larger and larger with the increase of twist

**Table 1** Knot complexities for Platonic and Archimedean polyhedral links

$T_{2k}$ -polyhedral links		$V$	$E$	$c(L)$	$u(D)$	$b(D)$
Platonic polyhedra	$T$ -links	4	6	$6k$	$3k$	$4 + 6(2k-1)$
	$O$ -links	6	12	$12k$	$6k$	$6 + 12(2k-1)$
	$C$ -links	8	12	$12k$	$6k$	$8 + 12(2k-1)$
	$I$ -links	12	30	$30k$	$15k$	$12 + 30(2k-1)$
	$D$ -links	20	30	$30k$	$15k$	$20 + 30(2k-1)$
Archimedean polyhedra	$Tt$ -links	12	18	$18k$	$9k$	$12 + 18(2k-1)$
	$Cu$ -links	12	24	$24k$	$12k$	$12 + 14(2k-1)$
	$To$ -links	24	36	$36k$	$18k$	$24 + 36(2k-1)$
	$Th$ -links	24	36	$36k$	$18k$	$24 + 36(2k-1)$
	$R$ -links	24	48	$48k$	$24k$	$24 + 48(2k-1)$
	$So$ -links	24	60	$60k$	$30k$	$24 + 60(2k-1)$
	$Id$ -links	30	60	$60k$	$30k$	$30 + 60(2k-1)$
	$Tcu$ -links	48	72	$72k$	$36k$	$48 + 72(2k-1)$
	$Ti$ -links	60	90	$90k$	$45k$	$60 + 90(2k-1)$
	$Td$ -links	60	90	$90k$	$45k$	$60 + 90(2k-1)$
	$Ri$ -links	60	120	$120k$	$90k$	$60 + 120(2k-1)$
	$Si$ -links	60	150	$150k$	$75k$	$60 + 150(2k-1)$
	$Tid$ -links	120	180	$180k$	$90k$	$120 + 180(2k-1)$

number  $k$ . For example, if  $k = 1$ , the braid index  $b(D)$  of the most complex polyhedral link  $T_2$ - $Tic$ -link is 300; whereas, if  $k = 26$ , the braid index  $b(D)$  of the least complex polyhedral link  $T_{52}$ - $T$ -link is 310. Clearly, the enough more twists a later link has, the more complex it is.

Since polyhedral links provide some appropriate mathematical frameworks for DNA polyhedral catenanes, our mathematical considerations offer a systematic analysis, as well as may open many possibilities to understand and control the molecular design and characterization. In fact, for chemical realization of DNA cages, the minimal number of circular DNA strands is another important quantity for detecting topological complexity. As promising developments, Jonoska et al. [48] and Grayson et al. [49] have found that this number for both dodecahedral and icosidodecahedral cages are two.

At the moment, however, there are many open problems appeared in the area of complexity of polyhedral links. They bring both challenges and opportunities including such as follows: (1) Compute more knot invariants to search for better topological indicators to guide the experiment. In particular, stick number becomes a natural measure since DNA strands can be considered as some rigid sticks. (2) Determine the complexity of topological constructions which are more complex than  $T_{2k}$ -polyhedral links. For instance, some constructions whose vertices are separated by odd numbers of DNA half-turns or edges are multi-crossover DNA molecules have been chemically realized and provide us research targets. (3) How the underlying principle of com-

plexity relates to physico-chemical properties of DNA polyhedra, as electrophoretic mobility in solution for example.

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